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The Schrödinger-Like Equation for a Nonrelativistic Electron in a Photon Field of Arbitrary Intensity

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(**Abstract**) The ordinary Schrödinger equation with minimal coupling for a nonrelativistic electron interacting with a single-mode photon field is not satisfied by the nonrelativistic limit of the exact solutions to the corresponding Dirac equation. A Schrödinger-like equation valid for arbitrary photon intensity is derived from the Dirac equation without the weak-field assumption. The "eigenvalue" in the new equation is an operator in a Cartan subalgebra. An approximation consistent with the nonrelativistic energy level derived from its relativistic value replaces the "eigenvalue" operator by an ordinary number, recovering the ordinary Schrödinger eigenvalue equation used in the formal scattering formalism. The Schrödinger-like equation for the multimode case is also presented.

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The exact analytical solutions for an electron interacting with a photon field play a very important role in theories and calculations of multiphoton ionization (MPI) and multiphoton scattering processes [1-8]. These theoretical results have achieved notable agreements [2,4,8] with experiments done during late 1980s [9-11]. However, rigorously speaking, the theoretical treatments for a nonrelativistic (NR) electron interacting with a photon field [3-6] had a logical loophole; the purpose of this note is to fill this loophole. A bonus of our efforts is the derivation of a Schrödinger-like equation for an NR electron interacting with a photon field that is valid for arbitrary photon intensity (within the range consistent with the NR motion of the electron).

Before proceeding to formal considerations, let us first point out an important feature of the MPI phenomenon. Namely, the total energy of the photons interacting with the electron in a strong radiation field can be comparable to the electron mass. For example, the photon energy of 1064 nm is of the order 1 eV, when the laser intensity is of the order 10^{13} $watt/cm^2$, the ponderomotive number is of order of unity. This number is the photon number in a disc volume V_p with thickness as the electron classical radius r_c and the cross section made by the radius of the photon circular wavelength $\lambda/2\pi$. The interaction volume of an atomic electron V can be regarded as a disk volume with the thickness as the Bohr radius and the same cross section of V_p. Thus, $V = 137^2 V_p$. At the mentioned intensity the background photon number is about 2×10^4 with total energy of the order 2×10^4 eV. If one increases the intensity of the light with the same wavelength to 2.5×10^{14} $watt/cm^2$, the total interacting background photon energy will be around the electron mass. So the weak-field approximation used in the usual quantum electrodynamics does not apply here. We are confronting the problem to get a non-relativistic approximation with arbitrary photon intensity. The problem addressed in this paper is realistic and in the range of current experiments.

The previous treatments [3-8] of the MPI theory adopt a second-quantized formulation for the laser field. The equations of motion, in the Heisenberg picture, for a relativistic (first-quantized) electron interacting with a photon field is the well-known Dirac equation which, say for the case of a single-mode laser, reads

$$[i\gamma\partial - e\gamma A(kx) - m_e]\Psi(x) = 0, \tag{1}$$

where

$$A(kx) = g(\epsilon a e^{-ikx} + \epsilon^* a^\dagger e^{ikx}), \tag{2}$$

with a and $a^\dagger$, respectively, the photon annihilation and creation operator, and $g = (2V_\gamma\omega)^{-1/2}$, V_γ being the normalization volume of the photon field, and the polarization four-vector $\epsilon = (0, \boldsymbol{\epsilon})$. The Dirac equation has been solved exactly either with a single-mode photon field [1] or with a multimode photon field which propagates in one direction [7]. The NR limit of these exact solutions has been derived in ref. [2], and one is tempted to use them in the the theory for MPI in which the emitted electrons are nonrelativistic.

As usual, the MPI theory started with the ordinary Schrödinger equation with the standard minimum coupling [12], which in the Schrödinger picture was the eigenvalue equation

$$H\Psi(\mathbf{r}) = \mathcal{E}\Psi(\mathbf{r}), \tag{3}$$

with the Hamiltonian

$$H = \frac{1}{2m_e}[-i\nabla - e\mathbf{A}(-\mathbf{k}\cdot\mathbf{r})]^2 + \omega N_a, \tag{4}$$

where

$$\mathbf{A}(-\mathbf{k}\cdot\mathbf{r}) = g(\boldsymbol{\epsilon} e^{i\mathbf{k}\cdot\mathbf{r}} a + \boldsymbol{\epsilon}^* e^{-i\mathbf{k}\cdot\mathbf{r}} a^\dagger), \tag{5}$$

and $g = (2V_\gamma\omega)^{-1/2}$, V_γ being the normalization volume of the photon field. N_a is the photon number operator:

$$N_a = \frac{1}{2}(aa^\dagger + a^\dagger a). \tag{6}$$

The polarization vectors $\boldsymbol{\epsilon}$ and $\boldsymbol{\epsilon}^*$ are defined by

$$\boldsymbol{\epsilon} = [\boldsymbol{\epsilon}_x \cos(\xi/2) + i\boldsymbol{\epsilon}_y \sin(\xi/2)]e^{i\Theta/2},$$
$$\boldsymbol{\epsilon}^* = [\boldsymbol{\epsilon}_x \cos(\xi/2) - i\boldsymbol{\epsilon}_y \sin(\xi/2)]e^{-i\Theta/2}, \tag{7}$$

and satisfy

$$\boldsymbol{\epsilon} \cdot \boldsymbol{\epsilon}^* = 1, \quad \boldsymbol{\epsilon} \cdot \boldsymbol{\epsilon} = \cos\xi e^{i\Theta}, \quad \boldsymbol{\epsilon}^* \cdot \boldsymbol{\epsilon}^* = \cos\xi e^{-i\Theta}.$$

The angle ξ determines the degree of polarization, such that $\xi = \pi/2$ corresponds to circular polarization and $\xi = 0$, to linear polarization. (The phase angle $\Theta/2$ is introduced to characterize the initial phase value of the photon mode in an earlier work [3]. With this phase, a full "squeezed light" transformation [13] can be fulfilled in the solution process. In multimode cases, the relative value of this phase for each mode will be important.)

In the following, we first show that the Schrödinger eigenvalue equation (3) with the NR Hamiltonian (4) is not satisfied by the NR wavefunctions obtained from the exact solutions to the corresponding Dirac equation (1). To see this, let us remove the coordinate dependence of the $\mathbf{A}(-\mathbf{k}\cdot\mathbf{r})$ field by applying a canonical transformation [14,15]

$$\Psi(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{r}N_a}\phi(\mathbf{r}). \tag{8}$$

Equation (3) then becomes

$$\{\frac{1}{2m_e}(-i\nabla - \mathbf{k}N_a)^2 - \frac{e}{2m_e}[(-i\nabla)\cdot\mathbf{A} + \mathbf{A}\cdot(-i\nabla)]$$
$$+\frac{e^2\mathbf{A}^2}{2m_e} + \omega N_a\}\phi(\mathbf{r}) = \mathcal{E}\phi(\mathbf{r}), \tag{9}$$

where $\mathbf{k}\cdot\mathbf{A} = 0$ by transversality. Here, $\mathbf{A}$ is coordinate-independent and defined as

$$\mathbf{A} = e^{i\mathbf{k}\cdot\mathbf{r}N_a}\mathbf{A}(-\mathbf{k}\cdot\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}N_a} = g(\boldsymbol{\epsilon}a + \boldsymbol{\epsilon}^* a^\dagger). \tag{10}$$

Setting $\phi(\mathbf{r}) = e^{i\mathbf{p}\cdot\mathbf{r}}\phi$, we obtain the coordinate-independent equation:

$$[\frac{1}{2m_e}(\mathbf{p} - \mathbf{k}N_a)^2 - \frac{e}{m_e}\mathbf{p}\cdot\mathbf{A} + \frac{e^2\mathbf{A}^2}{2m_e} + \omega N_a]\phi = \mathcal{E}\phi. \tag{11}$$

Now we note that the term $(\mathbf{k}N_a)^2 \equiv \mathbf{k}N_a \cdot \mathbf{k}N_a$ in Eqs. (9) and (11) does not exist in the Dirac equation (1) and its squared form, which contain the creation and annihilation operators only up to quadratic terms. The exact solutions to the Dirac equation and their NR limit were obtained from the photon Fock states, i.e. the number states, by only "squeezed light" and "coherent light" transformations [1]. Any equation satisfied by these states can consist of operators a or $a^\dagger$ only up to quadratic ones. Thus, the known NR wavefunctions [16] do not satisfy the NR Schrödinger eigenvalue equation (3).

To justify the use of the NR wavefunctions, one of the authors has introduced a special ansatz [3] which allows the replacement in Eq. (11) of the $\mathbf{k}N_a$ terms by $\kappa\mathbf{k}$ with κ a real number to be determined. The implicit assumption behind this ansatz is that the corrections caused by this replacement should be at most comparable to relativistic effects. With this ansatz and certain covariance requirements, the solutions turned out to be just the NR wavefunctions obtained by the NR limit from the exact solutions of the Dirac equations. Later, the ansatz was extended to the cases of multimode photon fields with multiple propagation directions [3,4,6]. Though this procedure leads to the correct NR wavefunctions in the single-mode case, the reasons why the ansatz works were not explained. Moreover, the validity of using the Schrödinger eigenvalue equation to describe an NR electron in a strong photon field and the validity of the ansatz in multimode cases have never been rigorously justified.

Unlike the classical-field treatment, where the light field is treated as an external field, our quantum field-theoretical approach for photons

requires a careful treatment to maintain relativistic invariance for the photon field, while only the electron is to be considered as an NR particle. The correct equation of motion should be derived from the Dirac equation in the Schrödinger picture:

$$(H_e + H_\gamma + V)\Psi(\mathbf{r}) = p_0\Psi(\mathbf{r}), \tag{12}$$

where

$$\begin{aligned} H_e &= \alpha \cdot (-i\nabla) + \beta m_e, \\ H_\gamma &= \omega N_a = \frac{\omega}{2}(aa^\dagger + a^\dagger a), \\ V &= -e\alpha \cdot \mathbf{A}(-\mathbf{k}\cdot\mathbf{r}), \end{aligned} \tag{13}$$

where $\Psi(\mathbf{r}) = \begin{pmatrix} \Psi_1(\mathbf{r}) \\ \Psi_2(\mathbf{r}) \end{pmatrix}$, and

$$\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \tag{14}$$

where $\Psi_1(\mathbf{r})$ and $\Psi_2(\mathbf{r})$ are the major and minor component respectively. Thus Eq. (12) can be written as

$$\begin{aligned} \sigma \cdot [-i\nabla - e\mathbf{A}(-\mathbf{k}\cdot\mathbf{r})]\Psi_2(\mathbf{r}) + (m_e + \omega N_a)\Psi_1(\mathbf{r}) &= p_0\Psi_1(\mathbf{r}), \\ \sigma \cdot [-i\nabla - e\mathbf{A}(-\mathbf{k}\cdot\mathbf{r})]\Psi_1(\mathbf{r}) + (-m_e + \omega N_a)\Psi_2(\mathbf{r}) &= p_0\Psi_2(\mathbf{r}). \end{aligned} \tag{15}$$

From the second equation of Eq. (15) we have

$$\Psi_2(\mathbf{r}) = (p_0 + m_e - \omega N_a)^{-1}\sigma \cdot [-i\nabla - e\mathbf{A}(-\mathbf{k}\cdot\mathbf{r})]\Psi_1(\mathbf{r}), \tag{16}$$

Substituting $\Psi_2(\mathbf{r})$ in the first equation of Eq. (15) and ignoring the term $\sigma \cdot [-e\mathbf{A}(-\mathbf{k}\cdot\mathbf{r})]\Psi_2(\mathbf{r})$ that pertains to the minor component, we obtain a solo equation for the major component

$$\{\sigma \cdot [-i\nabla - e\mathbf{A}(-\mathbf{k}\cdot\mathbf{r})]\}^2\Psi_1(\mathbf{r}) = [(p_0 - \omega N_a)^2 - m_e^2]\Psi_1(\mathbf{r}). \tag{17}$$

By neglecting the coupling between electron spin and photon polarization, i.e. the term of $[\sigma\cdot\boldsymbol{\epsilon},\sigma\cdot\boldsymbol{\epsilon}^*]$, we have (writing Ψ_1 as Ψ)

$$[-i\nabla - e\mathbf{A}(-\mathbf{k}\cdot\mathbf{r})]^2\Psi(\mathbf{r}) = [(p_0-\omega N_a)^2 - m_e^2]\Psi(\mathbf{r}). \tag{18}$$

This equation can be written as an eigenvalue-like equation

$$\{\frac{1}{2m_e}[-i\nabla - e\mathbf{A}(-\mathbf{k}\cdot\mathbf{r})]^2 + \omega N_a\}\Psi(\mathbf{r}) = \mathcal{E}(N_a)\Psi(\mathbf{r}), \tag{19}$$

with

$$\mathcal{E}(N_a) \equiv \frac{1}{2m_e}[(p_0-\omega N_a)^2 - m_e^2] + \omega N_a. \tag{19'}$$

Equation (19) can be solved exactly. The following are the main steps to obtain the solutions. The canonical transformation given by Eq. (7) removes the coordinate dependence. Thus the equation becomes

$$(-i\nabla - e\mathbf{A} - \mathbf{k}N_a)^2\phi(\mathbf{r}) = [(p_0-\omega N_a)^2 - m_e^2]\phi(\mathbf{r}). \tag{20}$$

By setting $\phi(\mathbf{r}) = e^{i\mathbf{p}\cdot\mathbf{r}}\phi$, we get the coordinate independent equation

$$[\mathbf{p}^2 - 2e\mathbf{p}\cdot\mathbf{A} + e^2\mathbf{A}^2 + 2(p_0\omega - \mathbf{p}\cdot\mathbf{k})N_a]\phi = (p_0^2 - m_e^2)\phi. \tag{21}$$

A "squeezed light" transformation

$$\begin{aligned} a &= \cosh\chi c + \sinh\chi e^{-i\Theta}c^\dagger, \\ a^\dagger &= \sinh\chi e^{i\Theta}c + \cosh\chi c^\dagger, \end{aligned} \tag{22}$$

and a "coherent light" transformation

$$\phi = D^\dagger \mid n\rangle_c, \qquad D = \exp(-\delta c^\dagger + \delta^* c), \tag{23}$$

$$\delta = eg\mathbf{p}\cdot\boldsymbol{\epsilon}_c{}^*/[(p_0\omega - \mathbf{p}\cdot\mathbf{k} + e^2g^2)^2 - e^4g^4\cos^2\xi]^{\frac{1}{2}},$$

can be introduced to simplify the equation. Finally we have exact solutions for the Schrödinger-like equation (19) or its equivalent form (18)

$$\Psi(\mathbf{r}) = V_e^{-\frac{1}{2}} \exp[i(-\mathbf{k}N_a + \mathbf{p}) \cdot \mathbf{r}] D^\dagger \mid n\rangle_c, \tag{24}$$

where

$$\mid n\rangle_c = \frac{c^{\dagger n}}{\sqrt{n!}} \mid 0\rangle_c,$$

$$\mid 0\rangle_c = (\cosh\chi)^{-\frac{1}{2}} \sum_{s=0}^{\infty} (\tanh\chi)^s (\frac{(2s-1)!!}{(2s)!!})^{\frac{1}{2}} e^{-is\Theta} \mid 2s\rangle, \tag{25}$$

$$\chi = -\frac{1}{2}\tanh^{-1}(\frac{e^2 g^2 \cos\xi}{p_0\omega - \mathbf{p}\cdot\mathbf{k} + e^2 g^2}).$$

Here $\mid 2s\rangle$ is the Fock state with $2s$ photons in the single-mode. The number p_0 is determined by the following algebraic equation

$$p_0^2 - m_e^2 = \mathbf{p}^2 + 2C(n+\frac{1}{2}) - 2e^2 g^2 (\mathbf{p}\cdot\boldsymbol{\epsilon}_c)(\mathbf{p}\cdot\boldsymbol{\epsilon}_c^*) C^{-1},$$

$$\tag{26}$$

$$C \equiv [(p_0\omega - \mathbf{p}\cdot\mathbf{k} + e^2 g^2)^2 - e^4 g^4 \cos^2\xi]^{\frac{1}{2}}.$$

The solutions are also the eigenfunction of the momentum operator:

$$(-i\nabla + i\mathbf{k}N_a)\Psi(\mathbf{r}) = \mathbf{p}\Psi(\mathbf{r}), \tag{27}$$

which shows that $\mathbf{p}$ is the total momentum of this system. The total momentum $\mathbf{p}$ has a unique decomposition on the electron mass shell with light-like component in the $\mathbf{k}$ direction [1,5]:

$$\mathbf{p} = \mathbf{P} + \kappa\mathbf{k},$$

$$p_0 = m_e + \frac{\mathbf{P}^2}{2m_e} + \kappa\omega, \tag{28}$$

$$\kappa = \frac{C(n+\frac{1}{2})}{m_e\omega} - \frac{e^2g^2(\mathbf{P}\cdot\boldsymbol{\epsilon}_c)(\mathbf{P}\cdot\boldsymbol{\epsilon}_c^*)}{m_e\omega C},$$
$$\to (n+\frac{1}{2}+u_p), \quad \text{(in the strong laser field case)}$$

with replacing $p_0\omega - \mathbf{p}\cdot\mathbf{k}$ by $m_e\omega$ in C. Here u_p is the ponderomotive energy in units of photon energy. With the help of Eq. (28), the solutions can be expressed as

$$\Psi(\mathbf{r}) = V_e^{-1/2} exp[i(-\mathbf{k}N_a + \mathbf{P} + \kappa\mathbf{k})\cdot\mathbf{r}]D^\dagger \mid n\rangle_c. \tag{29}$$

This result agrees with the known NR limit [2] of the exact solutions to the Dirac equation (1), because of the following relation in the NR limit:

$$p_0\omega - \mathbf{p}\cdot\mathbf{k} = (m_e + \frac{\mathbf{P}^2}{2m_e})\omega - \mathbf{P}\cdot\mathbf{k}$$
$$\to m_e\omega. \tag{30}$$

This provides us a consistency check for our equations (19) and (19′).

We emphasize that the Schrödinger-like equation (19) that we have derived in the NR limit is not an ordinary eigenvalue equation, since "eigenvalue" (19′) is an operator (rather than a real number), which is a quadratic element in the commuting subalgebra generated by N_a in the enveloping algebra of a and $a^\dagger$. This subalgebra is also called a Cartan subalgebra.

Though our Eq. (19) has the satisfying feature that the known NR wavefunctions solve it exactly, it does not fit well the formal scattering formalism which requires the wave functions to satisfy a true eigenvalue equation. We propose to resolve this problem, by numerizing the "eigenvalue" operator to its stationary values. In quantum mechanics, one can obtain the energy eigenvalues of a quantum system by the variational method. Actually all the eigenvalues are stationary values of the operator, not necessarily the minimum value except for

the ground state. Here we do not need any variational method since the wave functions are exactly known. In the following we show that the stationary values of the operator $\mathcal{E}(N_a)$ do give the correct energy levels of the NR system. By setting

$$\frac{d\mathcal{E}(N_a)}{d(\omega N_a)} = 0, \tag{31}$$

and treating $\mathcal{E}(N_a)$ as a function of ωN_a we find that the stationary value, at $\omega N_a = (p_0 - m_e)I$ with I being the identity operator, is

$$\mathcal{E}(N_a) \equiv (p_0 - m_e)I + \frac{1}{2m_e}(p_0 - m_e - \omega N_a)^2 \to \mathcal{E}I, \tag{32}$$

with

$$\mathcal{E} \equiv p_0 - m_e = \frac{\mathbf{P}^2}{2m_e} + \kappa\omega, \tag{32$'$}$$

which is nothing but the energy level [2] for the interacting system of the NR electron and the photon field without including the rest mass of the electron. The omission of the quadratic term in Eq. (32) is a NR limit process. We also observe that by replacing $N_a\omega$ in Eq. (19$'$) either by $\kappa\omega$ or by $(n+1/2)\omega$, $\mathcal{E}$ has the same value within the tolerance of the NR limit, showing the stationary nature of the value (32). With the replacement of the "eigenvalue" operator by its stationary value (32') in the eigenvalue-like equation (19), we get an effective eigenvalue equation, which just recovers the ordinary Schrödinger eigenvalue equation (3) with the minimal-coupling Hamiltonian (4). It is this effective Schrödinger equation together with the NR wavefunctions (24) that were used in the previous treatments [3-8]. So the physical predictions obtained there remain valid.

In this way, we are led to the following procedure for treating an NR electron in a photon field, which could be generalized to the cases of multimode and multipotentials:

(1) Solve the Schrödinger-like "eigenvalue" equation (19) to obtain the wavefunctions.

(2) Obtain the stationary values of the "eigenvalue" operator as the energy levels.

(3) Replace the operator "eigenvalue" by its stationary value to obtain an effective Schrödinger eigenvalue equation to be used in the formal scattering formalism.

In ending this article, we present the Schrödinger-like equation for an NR electron in a two-mode photon field for future studies as follows

$$\{\frac{1}{2m_e}[-i\nabla - e\mathbf{A}_1(-\mathbf{k}_1\cdot\mathbf{r}) - e\mathbf{A}_2(-\mathbf{k}_2\cdot\mathbf{r})]^2$$

$$+\omega_1 N_1 + \omega_2 N_2\}\Psi(\mathbf{r}) = \mathcal{E}(N_1, N_2)\Psi(\mathbf{r}), \tag{33}$$

$$\mathcal{E}(N_1, N_2) \equiv \frac{1}{2m_e}[(p_0 - \omega_1 N_1 - \omega_2 N_2)^2 - m_e^2] + \omega_1 N_1 + \omega_2 N_2.$$

The coordinate independent equation to solve is

$$[(\mathbf{p} - e\mathbf{A})^2 + 2p(k_1 N_1 + k_2 N_2) + 2e(\mathbf{k}_1 N_1 + \mathbf{k}_2 N_2)\cdot\mathbf{A}$$

$$-2k_1 k_2 N_1 N_2]\phi = (p_0^2 - m_e^2)\phi, \tag{34}$$

where $pk_i \equiv (p_0\omega_i - \mathbf{p}\cdot\mathbf{k}_i), (i = 1, 2)$ and $k_1 k_2 \equiv (\omega_1\omega_2 - \mathbf{k}_1\cdot\mathbf{k}_2)$.

Compared with Eq. (21), we see that this equation contains a higher order operator term $N_1 N_2$. Searching for solutions to this equation is one of our targets in the future research.

To summarize, in this paper we have addressed carefully the problem of the equations of motion for a nonrelativistic electron interacting with a single-mode photon field, which is valid for arbitrary photon intensity. We first showed that the usual Schrödinger eigenvalue equation is not solved by the NR limit of the wavefunctions that exactly solve the corresponding Dirac equation. Then a Schrödinger-like equation is

derived from the Dirac equation without using the weak-field assumption. Though the "eigenvalue" is an operator in a Cartan subalgebra involving the photon number operator, the new equation has a simpler structure compared to the usual eigenvalue equation. An effective Schrödinger equation with ordinary eigenvalues, good in the NR limit, is achieved by replacing the "eigenvalue" operator by a number, which then can be used in the formal scattering theory. The Schrödinger-like equation for the multi-mode case is also presented.

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16. Those who are curious about the explicit form of the NR wavefunctions are advised to take a look at Eq. (24) or (29), which coincides with the NR limit of the exact solutions to the Dirac equation (1).